Adaptive SINDy framework for constructing POD temporal modes

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1. Introduction

The SINDy methodology employs sparse regression to uncover complex system dynamics accurately. Within this framework, the introduction of the L1 norm enforces sparsity in optimizing the coefficient matrix alongside the inclusion of a lambda factor (λ). Concurrently, the Proper Orthogonal Decomposition (POD) method decomposes high-dimensional data into dominant spatial and temporal modes. The integration of SINDy and POD, termed SINDy-POD, enriches our understanding of system evolution by interpreting POD's temporal modes. Notably, the efficacy of SINDy hinges on judicious lambda factor selection prior to optimization, profoundly influencing the prediction of non-zero potential functions. Our project aims to integrate an adaptive lambda factor into the SINDy framework, streamlining the identification process of potential functions and eliminating the need for prior lambda knowledge. Leveraging the PyTorch package, we anticipate this enhancement will broaden the framework's applicability, effectively addressing a wider range of complex problems.

2. Methods

2.1 SINDy -POD Methodology

The SINDy methodology is a data-driven modeling technique aimed at uncovering the underlying dynamics of complex systems. It involves collecting system data and selecting a library of potential polynomial functions (Θ). Sparse regression is then applied to identify the simplest combination of functions that accurately describe the system's behavior ($\dot{X}$). Within the SINDy framework, the introduction of the L1 norm enforces sparsity during the optimization of the coefficient matrix (Ξ), and the inclusion of a lambda factor (λ) further delineates the significance of the L1 norm during this process. Mathematically, the optimization problem is defined as below,

$$\dot{\mathbf{X}} = \mathbf{\Theta}(\mathbf{X})\ \mathbf{\Xi}$$

$$\boldsymbol{\xi_k} = \underset{\xi_k{}'}{\mathbf{argmin}} \left\| \dot{\boldsymbol{X}} - \boldsymbol{\Theta}(\boldsymbol{X})\ \boldsymbol{\xi_k}' \right\|_2 + \boldsymbol{\lambda} \left\| \boldsymbol{\xi_k}' \right\|_1$$

On the other hand, the Proper Orthogonal Decomposition (POD) method decomposes high-dimensional data (X) into spatial (U) and temporal (V) dominant modes through singular value decomposition. This technique retains the most significant spatial and temporal patterns in the data, providing a compact representation that captures the essential features of the system's behavior. By extracting these dominant modes, POD effectively reduces the dimensionality of the data while preserving its key characteristics, making it a valuable tool for analysis.

$$\mathbf{X} = \mathbf{U}\,\mathbf{\Sigma}\,\mathbf{V}^*$$

Recently, the integration of SINDy and POD, known as the SINDy-POD method, in which one utilizes SINDy to interpret the temporal modes extracted by POD, offers a deeper understanding of system evolution. This integration significantly enhances the effectiveness of the SINDy-POD method by adeptly capturing essential dynamics while simultaneously reducing unnecessary complex features.

2.2 Problem Description

In the present work, our objective is to introduce the lambda factor as a trainable parameter within the SINDy framework, in addition to the coefficient matrix. This modification offers two primary advantages. Firstly, it alleviates the requirement for optimal initialization prior to optimization, which is essential for identifying parsimonious mathematical functions. Secondly, it eliminates the need for iterative optimization across various lambda values to discern commonly converged terms relevant to the system dynamics under investigation. For a given trainable lambda, two possibilities are considered: a scalar lambda (λ_{scalar}) variable that scales the entire coefficient matrix and a matrix lambda (λ_{matrix}) that maps to each element in the coefficient matrix. In total, the following four distinct lambda scenarios are examined to assess the efficacy of the proposed adaptive lambda in enhancing the SINDy performance during the system identification process.

- Zero lambda parameter: it imposes no L1 norm in the SINDy equation.
- Fixed scalar lambda parameter: an initial value is assumed and remains fixed during optimization.
- Adaptive scalar lambda parameter: an initial scalar value is assumed but adjusts dynamically during optimization.
- Adaptive matrix lambda parameter: an identity matrix is initialized and dynamically updated during optimization.

Here, we employ ground truth CFD data depicting transient blood flow through a symmetric stenosed coronary artery. To extract the desired POD modes, we focus on the post-stenotic velocity flowfield, which encapsulates all the complex flow features observed over a cardiac cycle. Subsequently, we utilize these temporal modes to assess the ability of the SINDy framework to identify the time evolution of blood flow data.

2.3 PyTorch Platform

The adaptive SINDy framework is developed in Python and leverages the PyTorch package widely used in the machine learning community. Across all four scenarios, we employ the Adam optimizer to train both the coefficient matrix and the adaptive lambda in the SINDy equation. This training process utilizes a step-decay variant of the dynamic learning rate for enhanced performance.

3. Results

3.1 Ground truth for SINDy framework

First, the transient post-stenotic flow fields of velocity magnitude are normalized across the entire cardiac cycle, consisting of 100-time instants. Subsequently, the POD technique is applied to the normalized velocity magnitude data to compute the spatial and temporal dominant modes. The outcomes of the POD analysis are illustrated in Fig. 1. Since an economic SVD is employed, the cumulative energy plot indicates that all POD modes are necessary for the accurate reconstruction of the flow fields. However, for our SINDy investigation, we focus on the temporal POD modes. Specifically, we utilize the first three dominant temporal modes displayed in Fig. 1 to examine their interactions within the proposed adaptive SINDy framework.

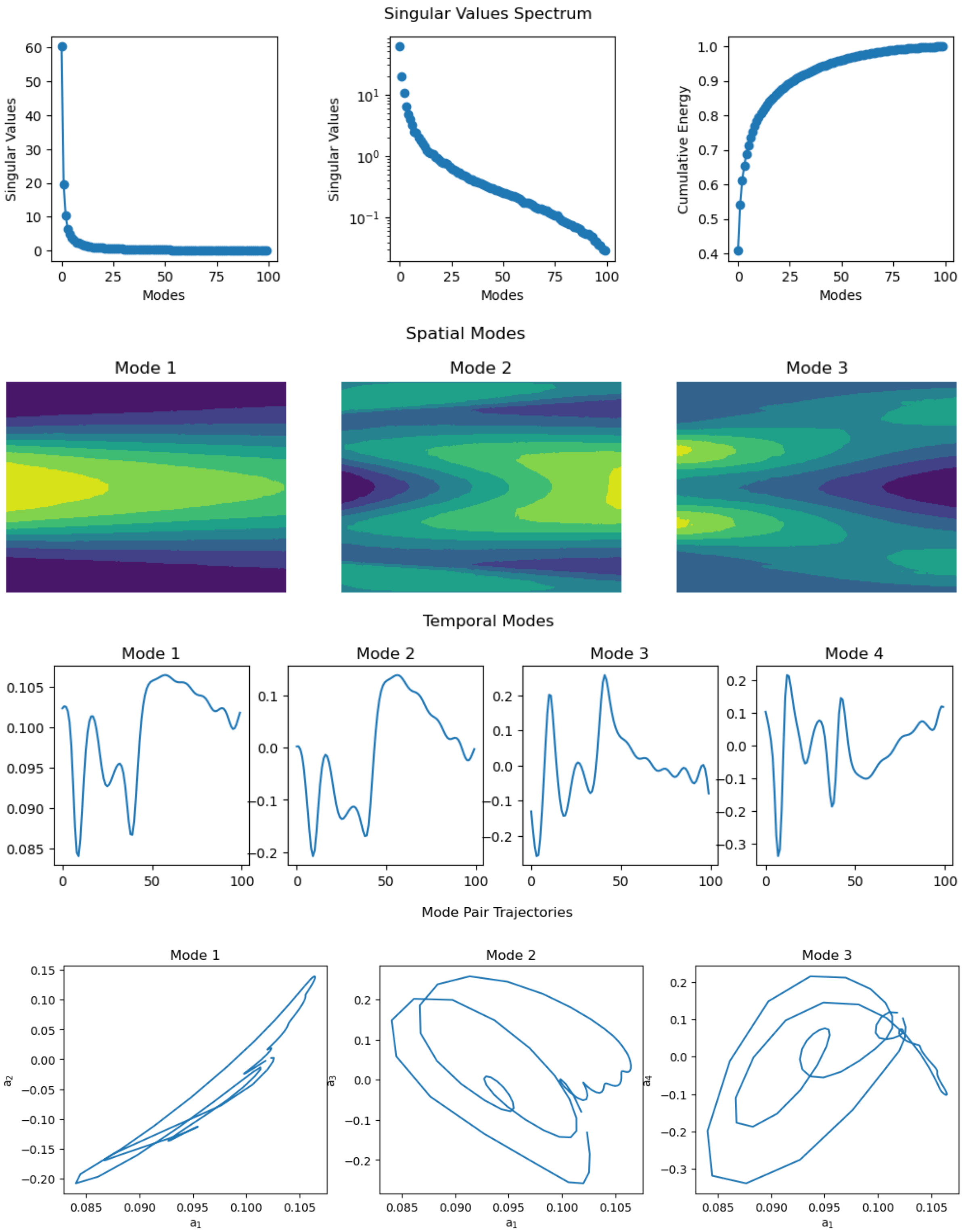

Fig. 1. Spatial and temporal POD modes extracted from the post-stenotic velocity flow field of the symmetrically stenosed coronary artery. (a) First row: showing the distribution of singular value across different modes. (b) Second row: depicting the first three dominant spatial modes. (c) Third row: representing the first four temporal modes. (d) Fourth row: indicating the mode pair trajectories.

3.2 Adaptive SINDy framework

To model the evolution of the three selected POD temporal modes, we employ the SINDy framework with potential polynomial functions up to the second order across four proposed lambda scenarios. In the second and third cases, lambda is initialized with a smaller value of $\mathbf{10^{-2}}$ before the optimization process. For the last matrix lambda variant, we begin with an **identity matrix**, as it corresponds to each element in the coefficient matrix. The total loss incurred in the four lambda scenarios is depicted in Fig. 2. While the zero lambda case demonstrates superior loss compared to the other scenarios, the crucial consideration lies in selecting the lambda variant strategy and its corresponding optimized coefficient matrix based on the achieved sparsity level, ensuring an effective capture of the system dynamics.

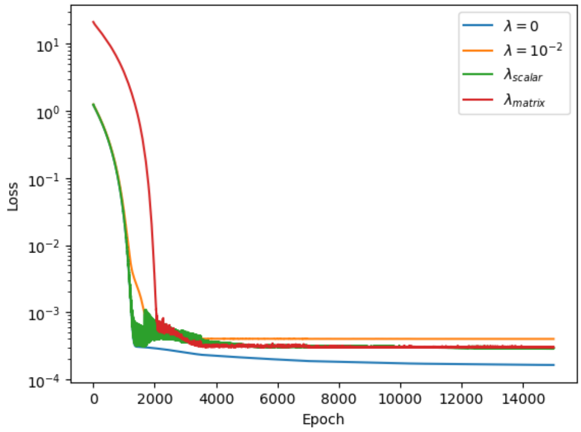

Fig. 2. Total loss incurred in optimizing the SINDy framework for the four different variants of lambda parameter.

The spectrum of the optimized coefficient matrix for the four lambda cases is depicted in Fig. 3. A threshold value of 0.001 centered at zero is chosen to eliminate the potential functions further due to negligible contribution in the converged SINDy model. Among the four lambda cases, it is apparent that the zero-valued lambda does not discriminate between the given potential functions, assuming that all candidates contribute equally. However, in the adaptive scalar lambda case, the sparsity level is significantly improved compared to the zero-valued case. Interestingly, both the fixed and matrix lambda variants perform exceptionally well, achieving the highest sparsity level in the coefficient matrix and retaining only a few potential terms. Notably, the sparsity level in the fixed lambda case is higher than in the matrix lambda case. The comparison of the adaptive SINDy-modeled temporal POD modes with the ground truth data is illustrated in Fig. 4. Comparing the two lambda methods, the SINDy framework adopting the adaptive matrix lambda faithfully reproduces the first two temporal POD modes compared to the fixed lambda method. However, for the last temporal POD mode, both lambda strategies fail to capture the high-frequency information in the given signal.

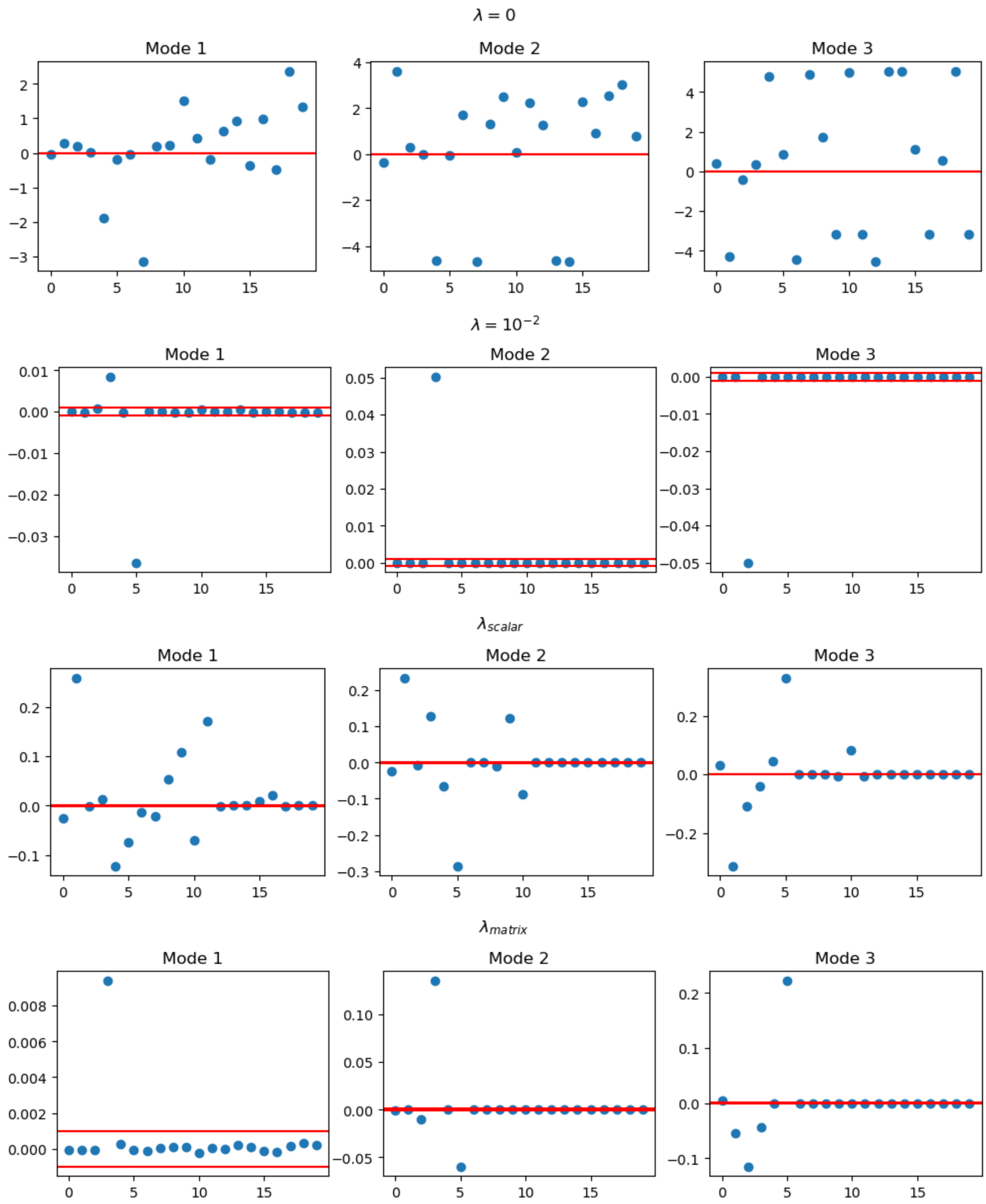

Fig. 3. Optimized coefficient matrix of the adaptive SINDy framework is presented for the four considered lambda variants. (a) First row: zero-valued lambda. (b) Second row: fixed scalar lambda. (c) Third row: adaptive scalar lambda. (d) Fourth row: adaptive matrix lambda.

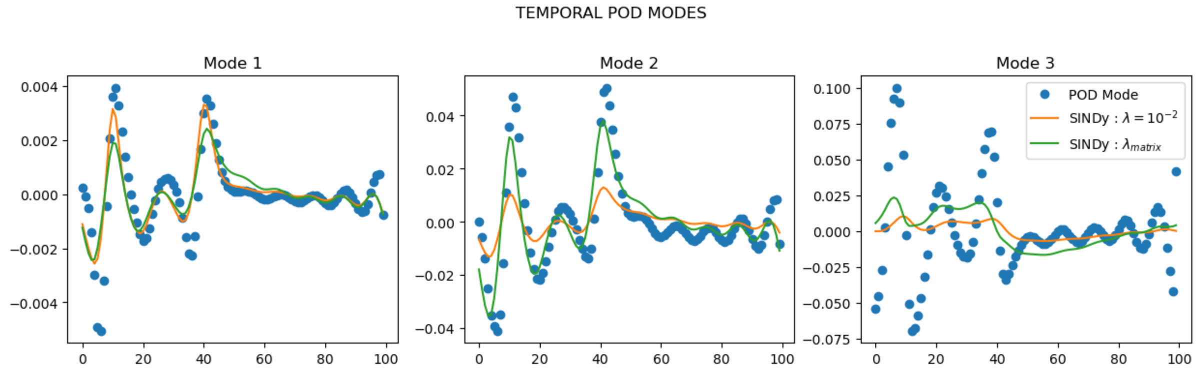

Fig. 4. Comparison of the first three modeled temporal POD modes using the adaptive SINDy framework with fixed and matrix lambda strategies against the ground truth data.

4. Discussion

In this project, we aimed to refine the SINDy framework by exploring its efficacy in modeling temporal POD modes using various L1 norm strategies. We introduced a trainable lambda parameter associated with the L1 norm during the optimization process, thereby eliminating the need for iterative experimentation with different lambda values to accurately identify potential functions. As anticipated, setting the lambda parameter to zero resulted in the inclusion of numerous unnecessary candidates for modeling the dynamics. Conversely, employing the other three lambda methods notably enhanced the sparsity level of the coefficient matrix. In our presented results, we initialized the lambda value to a smaller value of $\mathbf{10^{-2}}$ for both fixed and scalar adaptive cases. It's important to emphasize that the initialized value significantly influences the number of potential candidates advocated for by the SINDy method. Notably, the outcomes are observed to be insensitive to the initialized values in the matrix adaptive lambda case. This underscores the superiority of the Adaptive SINDy - matrix lambda approach over the conventional SINDy methodology. In future work, enhancing the prediction of temporal modes could involve integrating Fourier terms along with learnable frequencies into the candidate matirx. This augmentation would assist the SINDy methodology in resolving high frequencies present in the given data. The preliminary results of Adaptive SINDy containing **only** the fundamental Fourier modes are depicted in Fig. 5. It is evident from the figure that the inclusion of Fourier terms significantly improves the prediction of the second and third temporal modes, as compared to Fig. 4.

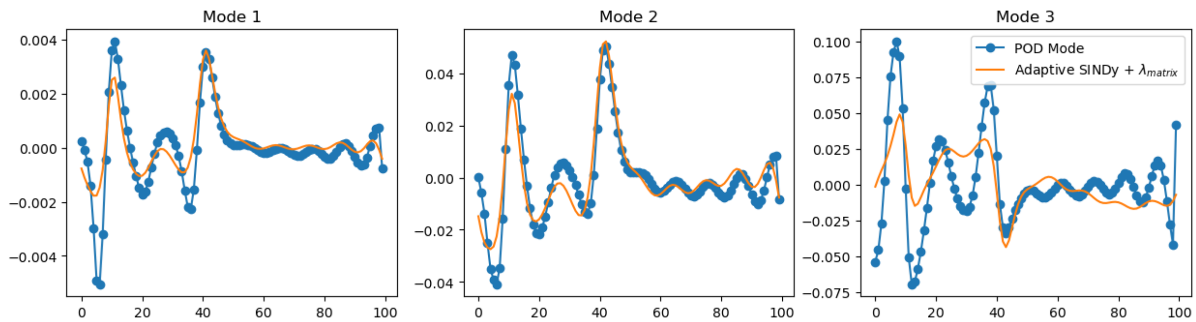

Fig. 5. Comparison of the first three modeled temporal POD modes using the adaptive SINDy framework with Fourier terms against the ground truth data.

5. Conclusion

In this project, we improved the SINDy methodology by introducing the lambda factor in L1 norm regularization as a trainable parameter. This adjustment yielded noteworthy improvements in identifying all three considered POD temporal modes, surpassing the performance of the fixed-valued lambda SINDy framework. Moreover, our observations indicate that incorporating Fourier terms with learnable frequencies into the candidate matrix yields substantial enhancements in accurately resolving the frequencies present in the data.